عنوان مقاله:

Theoretical investigation dielectric coefficient tautomerization process in gas and solution phase of 5-(x-amino)-1,3,4-(oxadiazol -2(3H)-one(x=Br

محل انتشار:

بیستمین کنگره شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Investigation of tautomerism and transition states in a derivative of 1,3,4-oxadiazole (A, B, C and D) In this combination of atomic bromine as halogen is used.in the gas and solution phase was performed by calculations at the DFT-B3LYP/6-311++G(d,p) level of theory. The geometries of four possible tautomers of 5-(x-amino)-1,3,4-oxadiazole-2(3H)-one were optimized in the gas and solution phase .It was found that in the gas and solution phase,transition states C D and A D tautomers are the most stable and unstable forms, respectively.The results show that the tautomeric interconversion C D has the lowest Gibbs free energy changes and so the highest equilibrium constant in the gas and water phase . The calculated results show that the highest rate k forward in the transition states C D In the substituent gas phase and lowest rate k forward in the transition states A D In the substituent Br in the water phase and highest rate k reverse in the transition states A D In the substituent Br in the gas phase and lowest rate k reverse in the transition states C D In the substituent Br in the solutuion phase

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا: